

Singular perturbations, regularization and extension theory

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For nonpositive singular potentials in quantum mechanics it can happen that the Schrödinger operator is not essentially self-adjoint on a natural domain of definition or not semibounded from below. In this case we have a lot of self-adjoint extensions each of them is a candidate for the right physical Hamiltonian of the system. Hence the problem arises to single out the right physical self-adjoint extension. Usually this problem is solved as follows. At first one has to approximate the singular potential by a sequence of bounded potentials (cut-off approximation). After that one has to show that the arising sequence of Schrödinger operators converges in the strong resolvent sense to one of the self-adjoint extensions if the cut-off approximation tends to the singular potential. The so determined self-adjoint extensions is regarded as the right physical Hamiltonian. Very often the right physical Hamiltonian coincides with the Friedrichs extension.

With respect to the Schrödinger operator in $L^2(\mathbf{R}^2)$ this problem was discussed by [3], [4], [5], [9] and [10]. An operator-theoretical investigation of this problem was started by Nenciu in [8] and continued by the authors in [7]. In the following we continue those abstract investigations. We assume that a semi-bounded symmetric operator admits a monotonously decreasing sequence of semi-bounded symmetric operators such that the corresponding sequence of Friedrichs extensions converges in the strong resolvent sense to the Friedrichs extension of the symmetric operator with which we have started. The problem will be to find necessary and sufficient conditions that any other sequence of semibounded self-adjoint extensions of the decreasing sequence of symmetric operators converges to this Friedrichs extension too. Unfortunately, we are unable to solve this problem in full generality. This means we have found a necessary condition which must be satisfied in order to have the desired convergence. However, we can prove the converse only for special sequences of self-adjoint extensions but not for all.

In more detail the problem can be described as follows. Let A and V be two nonnegative self-adjoint operators on the separable Hilbert space \mathcal{H} . Further, let $\mathcal{D} \subseteq \text{dom}(A) \cap \text{dom}(V)$ a dense subset of \mathcal{H} such that

$$(Vf, f) \leq a(Af, f) + b\|f\|^2, \quad f \in \mathcal{D}, \quad 0 < a, b. \quad (1)$$

We introduce the abstract operator \dot{H}_α

$$\dot{H}_\alpha f = Af - \alpha V f, \quad f \in \text{dom}(\dot{H}_\alpha) = \mathcal{D}, \quad \alpha > 0. \quad (2)$$

If the coupling constant α , $\alpha > 0$, obeys $\alpha < 1/a$, then the operator \dot{H}_α is symmetric, closable and semibounded with lower bound $-\alpha b$. However, the operator \dot{H}_α is in general not essentially self-adjoint.

Example 1 Let $\mathcal{H} = L^2(\mathbf{R}^1)$ and let A be the usual Laplace operator on $L^2(\mathbf{R}^1)$, i.e. $A = -d^2/dx^2$. By V we denote the multiplication operator arising from the real potential $V(x)$,

$$V(x) = \frac{1}{4\kappa} \frac{1}{|x|^\beta}, \quad 1 \leq \beta \leq 2, \quad \kappa > 0. \quad (3)$$

Let $\mathcal{D} = C_0^\infty(\mathbf{R}^1 \setminus \{0\})$. If $1 \leq \beta < 2$, then for every $\kappa > 0$ there are real numbers $a < 1$ and $b \geq 0$ such that

$$\int_{-\infty}^{\infty} \frac{1}{4\kappa} \frac{1}{|x|^\beta} |f(x)|^2 dx \leq a \int_{-\infty}^{\infty} |f'(x)|^2 dx + b \int_{-\infty}^{\infty} |f(x)|^2 dx. \quad (4)$$

for $\kappa > 0$. If $\beta = 2$, then this is only true for $\kappa > 1$.

Example 2 Let $\mathcal{H} = L^2(\mathbf{R}^2)$ and let A be the usual Laplace operator on $L^2(\mathbf{R}^2)$, i.e. $A = -\Delta$. Further, let Γ be a smooth curve in \mathbf{R}^2 which is parameterized by

$$\Gamma = \{(x, y) \in \mathbf{R}^2 : x = \rho(\varphi) \cos \varphi, y = \rho(\varphi) \sin \varphi, 0 \leq \varphi < 2\pi\} \quad (5)$$

where $\rho(\varphi) > 0$ is a smooth function. Again V is the multiplication operator arising from

$$V(x) = \frac{1}{5\kappa} \frac{1}{||x| - \rho(\varphi)|^\beta}, \quad 1 \leq \beta \leq 2, \quad |x| = \sqrt{x^2 + y^2}. \quad (6)$$

We set $\mathcal{D} = C_0^\infty(\mathbf{R}^2 \setminus \Gamma)$. If $1 \leq \beta < 2$, then for every $\kappa > 0$ there are real numbers $a < 1$ and $b \geq 0$ such that

$$\int_{\mathbf{R}^2} \frac{1}{5\kappa} \frac{1}{||x| - \rho(\varphi)|^\beta} |f(x)|^2 dx \leq a \int_{\mathbf{R}^2} |\nabla f(x)|^2 dx + b \int_{\mathbf{R}^2} |f(x)|^2 dx. \quad (7)$$

For $\beta = 2$ this is true only for $\kappa > 1$.

Let us assume that the \dot{H}_α is not essentially self-adjoint. Since \dot{H}_α is semibounded the Friedrichs extension \hat{H}_α exists. Moreover, denoting by \hat{A} the Friedrichs extension of $\dot{A} = A|_{\mathcal{D}}$ it is not hard to see that \hat{H}_α coincides with the form sum of \hat{A} and $-\alpha V$, i.e.

$$\hat{H}_\alpha = \hat{A} \dot{+} (-\alpha V). \quad (8)$$

In the above examples the Friedrichs extension corresponds to the Dirichlet boundary condition at $x = 0$ for the first example and on Γ for the second one.

Next let us introduce a regularizing sequence for the singular perturbation.

Definition 3 A sequence $\{V_n\}_{n \geq 1}$ of bounded non-negative self-adjoint operators is called a regularizing sequence of V if

- (i) $V_1 \leq V_2 \leq \dots \leq V_n \leq \dots \leq V$
- (ii) $\lim_{n \rightarrow \infty} (V_n f, f) = (V f, f)$, $f \in \mathcal{D} \subseteq \text{dom}(V)$.

Example 4 In the Examples 1 and 2 the sequence V_n is given as multiplication operators with the cut-off potentials

$$V_n(x) = \inf_{x \in \mathbf{R}^l} \{n, V(x)\}, \quad l = 1, 2. \quad (9)$$

With the regularizing sequence $\{V_n\}_{n=1}^\infty$ we associate the following sequence of self-adjoint operators $H_{\alpha,n}$,

$$H_{\alpha,n} = A - \alpha V_n, \quad n = 1, 2, \dots \quad (10)$$

The problem is now to find conditions which guarantee that the approximating sequence $\{H_{\alpha,n}\}_{n=1}^\infty$ tends to the Friedrichs extension \hat{H}_α , i.e.,

$$s - \lim_{n \rightarrow \infty} (H_{\alpha,n} - z)^{-1} = (\hat{H}_\alpha - z)^{-1}, \quad \Im(z) \neq 0 \quad (11)$$

However, from the mathematical point of view this setup seems to be unnatural. To explain this we remark that for any $n = 1, 2, \dots$ the operator $H_{\alpha,n}$ is a self-adjoint extension of the semibounded symmetric operator $\dot{H}_{\alpha,n} = H_{\alpha,n}|_{\mathcal{D}} = \dot{A} - \alpha V_n$, i.e. $\dot{H}_{\alpha,n} \subseteq H_{\alpha,n}$. Taking another semibounded self-adjoint extension \tilde{A} of \dot{A} we get another sequence $\tilde{H}_{\alpha,n}$,

$$\tilde{H}_{\alpha,n} = \tilde{A} - \alpha V_n, \quad n = 1, 2, \dots, \quad (12)$$

which naturally implies the question: why we should to investigate the convergence for $H_{\alpha,n}$ and why not for $\tilde{H}_{\alpha,n}$? So in the following we shall search for conditions which guarantee that

$$s - \lim_{n \rightarrow \infty} (\tilde{H}_{\alpha,n} - z)^{-1} = (\hat{H}_\alpha - z)^{-1}, \quad \Im(z) \neq 0. \quad (13)$$

for any semibounded self-adjoint extension \tilde{A} of \dot{A} . In particular, this would be clarified the uniqueness problem of the limit (13) for the two "extreme cases": the sequence of Friedrichs extension $\hat{H}_{\alpha,n}$,

$$\hat{H}_{\alpha,n} = \hat{A} - \alpha V_n, \quad n = 1, 2, \dots, \quad (14)$$

where \hat{A} is the Friedrichs extension of \dot{A} , and of the sequence of Krein extensions $\check{H}_{\alpha,n}$

$$\check{H}_{\alpha,n} = \check{A} - \alpha V_n, \quad n = 1, 2, \dots, \quad (15)$$

where \tilde{A} is the Krein extension (soft extension) [1], [2], [6] of \dot{A} with respect to a given lower bound $\eta < 0$, i.e. $\tilde{A} \geq \eta I$.

In general we cannot expect that the sequence $\tilde{H}_{\alpha,n}$ tends to \hat{H}_α assuming only that $\{V_n\}_{n \geq 1}$ is a regularizing sequence. Actually we need a little bit more. Only if \tilde{A} is the Friedrichs extension \hat{A} of \dot{A} , i.e. $\tilde{A} = \hat{A}$, then we obtain

$$s - \lim_{n \rightarrow \infty} (\hat{H}_{\alpha,n} - z)^{-1} = (\hat{H}_\alpha - z)^{-1}, \quad \Im(z) \neq 0, \quad (16)$$

without any additional assumptions [7]. How to find this additional assumptions? An essential hint comes from the following proposition.

Proposition 5 *Let $\{V_n\}_{n \geq 1}$ be a regularizing sequence of V . If for every self-adjoint extension \tilde{A} of $\dot{A} = A|_{\mathcal{D}}$ obeying $\tilde{A} \geq \eta$, $\eta < 0$, the convergence (13) takes place, then*

$$\sup_{n \geq 1} (V_n h, h) = +\infty \quad (17)$$

for every nontrivial h of $\mathcal{N}_\eta = \ker(\dot{A}^* - \eta)$.

By this proposition it seems to be natural to introduce the following notation.

Definition 6 Let $\{V_n\}_{n \geq 1}$ be a regularizing sequence of V . The sequence is called admissible with respect to $\dot{A} = A|_{\mathcal{D}}$ if there is a $\eta < 0$ such that for every nontrivial $h \in \mathcal{N}_\eta = \ker(\dot{A}^* - \eta)$ the condition (17) is satisfied.

Remark 7 It can be shown that if (17) is satisfied for one $\eta < 0$, then it holds for every $\eta' < 0$. So the property (17) is independent on $\eta < 0$.

Example 8 It can be shown that the regularizing sequences of Example 4 for the Examples 1 and 2 are admissible with respect to $\dot{A} = -\frac{d}{dx^2}|C_0^\infty(\mathbf{R}^1 \setminus \{0\})$ and $\dot{A} = -\Delta|C_0^\infty(\mathbf{R}^2 \setminus \Gamma)$.

Hence, the optimal way to solve our problem would be to show that the converse to Proposition 5 is true, i.e., if $\{V_n\}_{n \geq 1}$ is an admissible regularizing sequence of V with respect to $\dot{A} = A|_{\mathcal{D}}$, then for every semibounded self-adjoint extension \tilde{A} of \dot{A} we have that the convergence (13) is valid. Till now we cannot prove this conjecture in full generality. However, if we restrict the set of semibounded self-adjoint extensions \tilde{A} of \dot{A} , then we can do it. To describe these restrictions we use a description of all semibounded self-adjoint extensions which goes back to [1]. Let \tilde{A} be any semibounded self-adjoint extension of $\dot{A} = A|_{\mathcal{D}}$ with lower bound greater than $\eta < 0$, i.e. $\tilde{A} \geq \eta$. By $\tilde{\nu} \geq \eta$ we denote the closed quadratic form which corresponds to \tilde{A} , i.e.

$$\begin{aligned} \tilde{\nu}(f, f) &= ((\tilde{A} - \eta)^{1/2} f, (\tilde{A} - \eta)^{1/2} f) + \eta(f, f), \\ f \in \text{dom}(\tilde{\nu}) &= \text{dom}((\tilde{A} - \eta)^{1/2}). \end{aligned} \quad (18)$$

In particular, by $\hat{\nu} \geq 0$ we denote the closed quadratic form which corresponds to the Friedrichs extension \hat{A} of \dot{A} . In accordance with [1] we have an one-to-one correspondence between the set of all semibounded self-adjoint extensions \tilde{A} of \dot{A} obeying $\tilde{A} \geq \eta$ and all non-negative closed quadratic forms \tilde{q} on the deficiency subspace $\mathcal{N}_\eta = \ker(\dot{A}^* - \eta)$, where the form \tilde{q} is not necessarily densely defined on \mathcal{N}_η . The correspondence is given by the formulas

$$\text{dom}(\tilde{\nu}) = \text{dom}(\hat{\nu}) \dot{+} \text{dom}(\tilde{q}), \quad (19)$$

where $\dot{+}$ means $\text{dom}(\hat{\nu}) \cap \text{dom}(\tilde{q}) = \{0\}$, and

$$\tilde{\nu}(g + h, g + h) = \hat{\nu}(g, g) + \tilde{q}(h, h) + 2\eta\Re(g, h) + \eta(h, h), \quad (20)$$

$g \in \text{dom}(\hat{\nu}), h \in \text{dom}(\tilde{q}) \subseteq \mathcal{N}_\eta$. Therefore, starting with extension \tilde{A} which obeys $\tilde{A} \geq \eta$ we can find a unique non-negative closed quadratic form \tilde{q} on \mathcal{N}_η such that (19) and (20) holds. Conversely, if we have a non-negative closed quadratic form \tilde{q} on \mathcal{N}_η , then we can define by (19) and (20) a semibounded extension \tilde{A} of \dot{A} obeying $\tilde{A} \geq \eta$. The domain of \tilde{q} may be a closed subspace of \mathcal{N}_η or not. The Friedrichs extension \hat{A} corresponds to the trivial form \hat{q} , i.e., $\text{dom}(\hat{q}) = \{0\}$. Very often this is expressed by $\hat{q} = +\infty$. The Krein extension (soft extension) [1], [2], [6] \check{A} with respect to the lower bound $\eta < 0$, i.e. $\check{A} \geq \eta I$, is given by the form \check{q} which is zero on the whole deficiency subspace \mathcal{N}_η , i.e., $\check{q} = 0$. All other forms $\tilde{\nu}$ are between $\check{\nu}$ and $\hat{\nu}$ which yields $\check{A} \leq \tilde{A} \leq \hat{A}$.

Of course the description is only unique if we fix some $\eta < 0$. Changing η we get different quadratic forms \tilde{q}_η for the same semibounded self-adjoint extension \tilde{A} of \dot{A} . However, there are some invariants which do not depend on η . For instance, if $\text{dom}(\tilde{q}_\eta)$ is a closed subspace in \mathcal{N}_η , then $\text{dom}(\tilde{q}_{\eta'})$ is a closed subspace for $\eta' (< 0)$, too.

Using this description our main theorem can be formulated now as follows.

Theorem 9 *Let $\{V_n\}_{n \geq 1}$ be an admissible regularizing sequence of V with respect to \dot{A} and let \tilde{A} be a self-adjoint extension of \dot{A} obeying $\tilde{A} \geq \eta$ for some $\eta < 0$. If \tilde{A} corresponds to a closed quadratic form \tilde{q} on $\mathcal{N}_\eta = \ker(\dot{A}^* - \eta)$ and the domain $\text{dom}(\tilde{q})$ is a closed subspace of \mathcal{N}_η , then for sufficiently small coupling constants $\alpha > 0$ we have*

$$s - \lim_{n \rightarrow \infty} (\tilde{H}_{\alpha, n} - z)^{-1} = (\hat{H}_\alpha - z)^{-1}, \quad \Im m(z) \neq 0, \quad (21)$$

where \hat{H}_α is the Friedrichs extension of $\dot{H}_\alpha = (A - \alpha V)|_{\mathcal{D}}$.

In particular, if \check{A} denotes the Krein extension of \dot{A} with respect to the lower bound $\eta < 0$, then for sufficiently small $\alpha > 0$ we have

$$s - \lim_{n \rightarrow \infty} (\check{H}_{\alpha, n} - z)^{-1} = (\hat{H}_\alpha - z)^{-1}, \quad \Im m(z) \neq 0. \quad (22)$$

If the deficiency indices are finite, then the theorem admits a strengthening.

Theorem 10 *If the deficiency indices of \dot{A} are finite, then for any self-adjoint extension \tilde{A} of \dot{A} and any coupling constant $\alpha < 1/a$ we have (21).*

The Theorem 10 improves the results of Section 3 of [7]. Moreover, the theorem can be slightly generalized.

Corollary 11 *If \tilde{A} is a semibounded self-adjoint extension of \dot{A} such that*

$$\dim(\text{dom}(\tilde{v})/\text{dom}(\hat{v})) < +\infty, \quad (23)$$

then for $\alpha < 1/a$ (21) is valid.

The theorems and corollary admit an application to our examples.

Example 12 Since in Example 1 the deficiency indices of $\dot{A} = -\frac{d}{dx^2}|C_0^\infty(\mathbf{R}^1 \setminus \{0\})$ are finite by Corollary 10 we always have the desired convergence (21).

In Example 2 we have the desired convergence (21) only for a special set of self-adjoint extensions of $\dot{A} = -\Delta|C_0^\infty(\mathbf{R}^2 \setminus \Gamma)$. The set includes the Krein extension (the corresponding boundary condition can be found in [1]) and extensions which are characterized by Corollary 11. However, it remains an open question: whether the sequence of usual Schrödinger operators $H_{\alpha,n} = -\Delta - \alpha V_n$, where $-\Delta$ denotes the usual Laplace operator in $L^2(\mathbf{R}^2)$ converges to the Friedrichs extension of the symmetric operator $(-\Delta - \alpha V)|C_0^\infty(\mathbf{R}^2)$? The problem is that the domain of the closed quadratic form, which by (18) - (20) corresponds to the usual Laplace operator $-\Delta$ in $L^2(\mathbf{R}^2)$ regarded as a self-adjoint extension of $-\Delta|C_0^\infty(\mathbf{R}^2)$, is not a closed subspace in \mathcal{N}_η .

Remark 13 If the deficiency indices are finite, then the strong resolvent convergence (21) can be replaced by the operator-norm convergence [7]. However, if the deficiency indices are infinite this is not true in general. For instance, let in Example 2 the curve Γ be the unite circle. Then one can show that for any interval $\delta \subseteq (-\infty, 0)$ and any integer N there is a greater integer $n \geq N$ such that $H_{\alpha,n}$ has an eigenvalue in δ . Consequently, this excludes the operator-norm convergence for the operators $\{H_{\alpha,n}\}_{n \geq 1}$.

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